On the absence of the glass transition in two dimensional hard disks

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In this paper we study the glass transition in a model of identical hard spheres, focusing on the two dimensional case. In the mean-field limit the model exhibits an ideal glass transition of the same nature of that found in discontinuous spin glasses. Nevertheless, a systematic expansion around the mean-field solution seems to indicate that the glass transitions is smeared out in two dimensions, in agreement with some recent results. Our investigation could be generalized to higher spatial dimensions, providing a way to determine the lower critical dimensionality of the mean-field ideal glass picture.

Under fast enough cooling or densification diverse materials, such as molecular and polymeric liquids, colloidal suspensions, granular assemblies, molten mixtures of metallic atoms, may form glasses [1], i.e., amorphous states that may be characterized mechanically as a solid, but lack of the long range crystalline order. Despite all the work devoted to the subject, the underlining mechanisms responsible for the vitrification processes are not well understood, as the transition to the glassy state is still deemed specifically to be one of the most obscure enigmas in condensed matter physics. Many valuable theories attempt to describe these remarkable phenomena, but none of them is as yet regarded as compelling.

A system of identical hard spheres confined in a fixed volume [2, 3, 4, 5, 6, 7, 8, 9] is the simplest system exhibiting a dramatic slowing down of the dynamics in the high volume fraction region, referred by many authors as a glass transition [3, 4, 8, 9]. In a recent paper [8], using a replica approach it has been very nicely shown that hard spheres in large space dimensions undergo an ideal glass transition at a volume fraction ϕ_K. The same result has been obtained in three dimensions employing diverse kinds of mean-field-like approximations (such as the hypernetted chain approximation [9] and the small cage expansion [5, 8]) and using the Carnhan-Starling equation of state. However, for finite dimensional systems (with short range interactions) the mean-field picture should be modified by (non-perturbative) activated events [10], and one might wonder to what extent the mean-field scenario is still valid in that case.

Here we study a system of identical hard disks on a two dimensional square lattice. We first analyze the mean-field solution, where an ideal glass transition of the same nature of that found in mean-field model for glasses [11] occurs. We then consider a systematic expansion around the mean-field limit, which allows to take into account short range correlations as corrections to the mean-field approximation. This is accomplished by considering bigger two dimensional $L \times L$ square cells of size $L = 2, 3, \ldots$, within which the model is solved exactly (see also Ref. [12, 13]). We observe that the glass tran-

sition occurs at higher densities as the size of the cell is increased, and seems to be smeared out in the limit $L \to \infty$. This analysis hints that there is no glass transition in two dimensional hard disks, in agreement with the recent results of Refs. [5, 6, 7]. Interestingly enough, the study presented here could be easily generalized to higher spatial dimensions, providing a direct way to estimate the lower critical dimensionality of the mean-field ideal glass picture. The latter investigation could prune down the number of candidate theories for the glass transition.

The Hamiltonian of the model reads:

$$\mathcal{H} = \sum_{[i,j]} J\, n_i n_j, \tag{1}$$

where the lattice variables $n_i = 0, 1$ whether the cell i is occupied by a particle or not, and the sum is restricted over the couples of sites $[i,j]$ such that their distance is equal or less than two lattice spacings: $d_{i,j} \leq 2$. The model can be regarded as a system of hard disks of diameter $\sqrt{5} - \epsilon$ lattice spacings. The limit $J \to \infty$ is taken, insuring the hard core exclusion.

The model can be solved in mean-field on the random regular graph [14], i.e., a random lattice where every vertex has $k + 1$ neighbors, but which is otherwise random (to mimic the two dimensional case, we choose $k = 3$). Locally the graph has a tree-like structure with a finite branching ratio, but has loops of typical size $\ln N$. The presence of loops is crucial to insure the geometric frustration, but the local tree structure allows for an analytical solution of the model, since we can write down iterative equations on the local probability measure. To this aim, let us consider a branch of the tree ending on the site i, and denote by i_j, $j \in \{1, \ldots, k\}$, the roots of the branches connected to the site i. We call $Z_1^{(i)}$ the partition function of this branch restricted to the configurations where the site i is occupied by a particle. Analogously, we define $Z_0^{(i)}$ the partition function of the branch restricted to configurations where the site i is empty, and $\overline{Z}_0^{(i)}$ the partition function of the branch restricted to configurations where the site i is empty with all neighbors
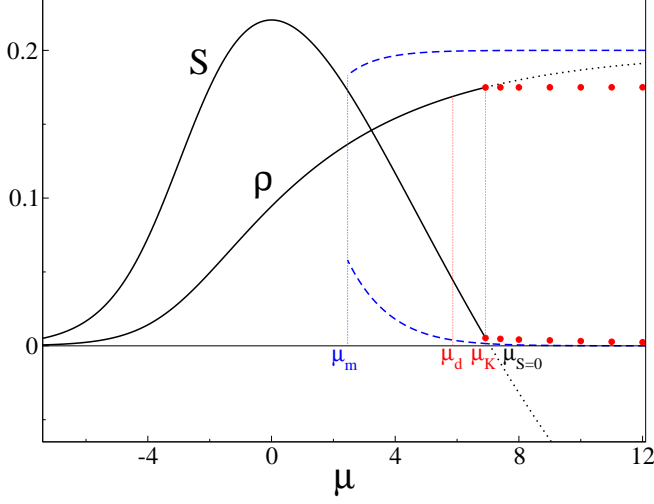
FIG. 1: Mean field solution of the model on the random graph. Density, ρ, and entropy per site, S, as a function of the chemical potential, μ, in the liquid (black continuous curve), crystalline (blue dashed curve), and glassy (red circles) phases.

i_j empty. Using the Grand Canonical ensemble, the following recursion relations are derived:

$$Z_1^{(i)} = e^{\beta\mu} \prod_{j=1}^{k} \overline{Z}_0^{(i_j)}, \qquad \overline{Z}_0^{(i)} = \prod_{j=1}^{k} Z_0^{(i_j)},$$

$$Z_0^{(i)} = \left[1 + \sum_{j=1}^{k} \frac{Z_1^{(i_j)}}{Z_0^{(i_j)}} \right] \prod_{j=1}^{k} Z_0^{(i_j)}, \qquad (2)$$

where μ is the chemical potential. It is convenient to introduce on any site i the local cavity fields $\beta h_i = \ln(Z_1^{(i)}/Z_0^{(i)})$ and $\beta v_i = \ln(\overline{Z}_0^{(i)}/Z_0^{(i)})$, in term of which the iteration relations, Eqs. (2), read:

$$e^{\beta h_i} = e^{\beta\mu + \sum_{j=1}^{k} \beta v_{i_j}} \left(1 + \sum_{j=1}^{k} e^{\beta h_{i_j}} \right)^{-1},$$

$$e^{\beta v_i} = \left(1 + \sum_{j=1}^{k} e^{\beta h_{i_j}} \right)^{-1}. \qquad (3)$$

From these fields one can obtain the free energy, $\beta F = -\ln Z$, as a sum of site and link contributions [14]: $F = \Delta F_s - (k+1)\Delta F_l/2$. The contribution from the bond between two branches with root sites i_1 and i_2 is:

$$e^{-\beta\Delta F_l} = 1 + e^{\beta(h_{i_1}+v_{i_2})} + e^{\beta(h_{i_2}+v_{i_1})}, \qquad (4)$$

while the contribution from the addition of a site i connected with $k+1$ branches with root sites i_j reads:

$$e^{-\beta\Delta F_s} = 1 + \sum_{j=1}^{k+1} e^{\beta h_{i_j}} + e^{\beta\mu + \sum_{i=1}^{k+1} \beta v_{i_j}}. \qquad (5)$$

Starting from Eqs. (3), we find at low density a liquid phase, characterized by a homogeneous (replica symmetric) solution, $h_i = h$ and $v_i = v$. Given this solution, using Eqs. (4) and (5), the thermodynamic quantities can be derived, and, in particular, the density $\rho = \langle n_i \rangle$ and the entropy per lattice site, $S = -\beta F - \beta\mu\rho$, are obtained (continuous curve in Fig. 1). As the chemical potential (the density) is increased, a first order phase transition from the liquid phase to a crystalline phase occurs at a melting point $\mu_m \simeq 2.46$ ($\rho_m \simeq 0.1364$). The crystalline state is characterized by a periodic structure, which breaks down the translational invariance, and can be obtained introducing different sub-lattices. More precisely, we introduce three sub-lattices, a, b, and c, on which the local cavity fields are site independent. The sub-lattices must be organized in such a way to reproduce the crystalline order: each vertex of the sub-lattice a is connected with 3 sites of the sub-lattice b [i.e., $a \to (b,b,b)$]. Analogously, we have $b \to (c,c,c)$ and $c \to (c,c,a)$. Also the free energy shifts, Eqs. (4) and (5), must be computed carefully, taking into account the structure of the three sub-lattices. In the crystalline phase, as the chemical potential is further increased above μ_m, the density rapidly approaches the maximum density, $\rho_{max} = 0.2$, and the entropy per site approaches zero (dashed curves in Fig. 1).

The crystallization transition can be avoided and, in this case, the system enters a supercooled state, still described by the homogeneous solution of Eqs. (3). However, as shown in Fig. 1, the entropy per site in the supercooled liquid becomes negative when the density is increased above $\rho_{S=0} \simeq 0.1757$ (or the chemical potential is increased above $\mu_{S=0} \simeq 7.07$). As a consequence, a thermodynamic phase transition must occur at a density $\rho \lesssim \rho_{S=0}$. In fact, in the mean-field approximation we find that the system undergoes a phase transition toward a 1RSB glassy phase, which can be analyzed by taking into account the existence of many different local minima (or pure states) of the free energy. Since in this case the local fields can fluctuate from pure state to pure state, this situation is described by a probability distribution $P(h,v)$ that the fields h_i and v_i on the site i equal h and v for a randomly chosen pure state. Using the cavity method [14] we find that this function satisfies the self-consistent equation:

$$\frac{P(h,v)}{\mathcal{N}e^{-\beta mv}} = \int \prod_{j=1}^{k} [dh_{i_j} dv_{i_j} P(h_{i_j}, v_{i_j})] \delta(h - h_i)\delta(v - v_i), \qquad (6)$$

where $\mathcal{N}$ is a normalization constant, h_i and v_i are the local cavity fields obtained when merging k branches which carry the fields (h_{i_j}, v_{i_j}) [via Eq. (3)], and $m \in [0,1]$ is a Lagrange multiplier which turns out to be the usual 1RSB parameter, fixed by the maximization of the free energy with respect to it [14, 15].

The 1RSB cavity equation, Eq. (6), can be solved exactly in the close packing limit ($\beta \to \infty$), where the re-
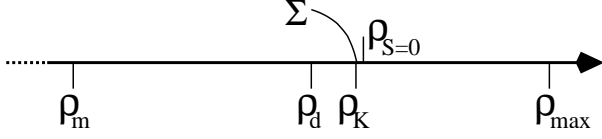
FIG. 2: Schematic drawing of the location of the relevant densities emerging from the mean-field solution: melting density, $\rho_m \simeq 0.1364$, dynamical transition density, $\rho_d \simeq 0.1688$, Kauzmann transition density, $\rho_K \simeq 0.1750$, density at which the entropy of the supercooled liquid vanishes, $\rho_{S=0} \simeq 0.1757(\sim \rho_K)$, maximum density of the crystalline packing, $\rho_{max} = 0.2$. The figure also show that the configurational entropy, Σ, defined as the logarithm of the number of pure states, is positive for $\rho_d \leq \rho \leq \rho_K$.

cursion relations, Eq. (3), simplify to:

$$h_i = 1 + \sum_j v_{i_j} - V(h_{i_j}), \qquad v_i = -V(h_{i_j}) \quad (7)$$

with $V(h_{i_j}) = \max\{h_{i_j}\}\theta(\max\{h_{i_j}\})$ [we have set $\mu = 1$]. These equations yield an exact ansatz for the cavity fields probability distribution: $P(h,v) = \sum_{r=1}^{7} p_r \delta(h - h_r)\delta(v - v_r)$, with $h_{1,2,3,4} = 1, 0, -1, -2$, $v_{1,2,3,4} = 0$, $h_{5,6,7} = 0, -1, -2$, and $v_{5,6,7} = -1$. By defining $P = p_1$, $R = p_2 + p_3 + p_4$, and $Q = p_5 + p_6 + p_7 = 1 - P - R$, Eq. (6) becomes:

$$P = R^3 \left[e^y - (e^y - 1)(1 - P)^3 \right]^{-1}, \quad (8)$$
$$R = \left[(1 - P)^3 - R^3 \right] \left[e^y - (e^y - 1)(1 - P)^3 \right]^{-1},$$

where $y = \lim_{\beta \to \infty} \beta m$. In terms of P and R, the 1RSB link and site contribution to the free energy read:

$$\Delta\phi_l[y] = -y^{-1}\ln\left\{ 1 + (e^y - 1)P^2 + 2e^y PR \right\} \quad (9)$$
$$\Delta\phi_s[y] = -y^{-1}\ln\left\{ e^y + (e^y - 1)\left[R^4 - (1 - P)^4 \right] \right\}.$$

The free energy is then given by $\phi[y] = \Delta\phi_s[y] - 2\phi_l[y]$, from which we can compute the complexity $\Sigma = y^2 \partial\phi[y]/\partial y$ and the density $\rho = \partial(y\phi[y])/\partial y$.

The finite μ solution of the 1RSB cavity equations can be found numerically, using the population dynamics algorithm [14]. In agreement with the results of Refs. [8, 9], the mean-field solution of the model exhibits an ideal glass transition of the same nature of that found in mean-field discontinuous spin glasses [11]. We first find a purely dynamical transition at $\rho_d \simeq 0.1688$ ($\mu_d \simeq 5.86$), where a non trivial solution of Eq. (6) appears for the first time, signaling the emergence of an extensive number of metastable states (which, in mean-field, trap the dynamics for an infinite time). A solution of the 1RSB equation becomes thermodynamically stable at a higher density, $\rho_K \simeq 0.1750$ ($\mu_K \simeq 6.92$), where a thermodynamic transition to a 1RSB glassy phase takes place. The relevant densities emerging from the mean-field approximation are reported in Fig. 2, showing that ρ_K is strikingly close to $\rho_{S=0}$.
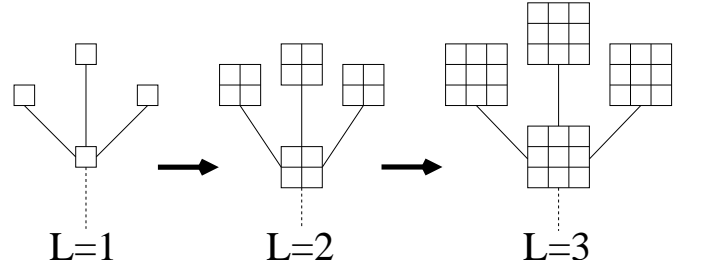

FIG. 3: Expansion around the mean-field solution. Starting from the mean-field limit ($L = 1$), bigger finite-dimensional cells of size $L = 2$ and $L = 3$ are considered.
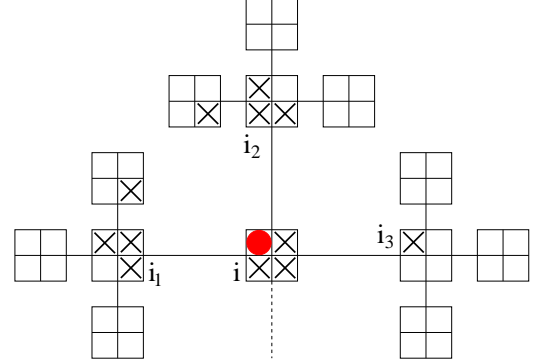

FIG. 4: Case $L = 2$: the figure depicts a configuration in which a particle (red circle) occupies one of the two forward sites of the branch ending on the cell i, i.e., one of the two sites which are not on the edge of the cell where the link is missing. The sites whose distance from the particle is less or equal than two lattice spacings cannot be occupied (these sites are marked by crosses).

In the following we consider a systematic expansion around the mean-field theory, which takes into account the actual structure of the two dimensional square lattice. More precisely, we consider cells of size $L = 2, 3$ within which the model is solved "exactly" and we use those cells as vertex of the mean-field theory on the random graph, as depicted in Fig. 3 (see also Refs. [12, 13]). In the limit $L \to \infty$ the exact solution of the model should be achieved. This method allows to include in an exact fashion short range spatial correlations, as correction to the mean-field limit. Since in glassy systems there is no diverging *equilibrium* length scale, this expansion is expected to be reliable and effective.

In order to solve the $L = 2$ case, let us consider a branch of the tree ending on the 2×2 square cell i, and denote by i_j, $j \in \{1, \ldots, k\}$, the roots of the branches connected to the cell i, as shown in Fig. 4. We call $U^{(i)}$ (resp., $D^{(i)}$) the partition function of the branch restricted to the configurations in which the cell is occupied by a particle in one of the two "forward" (resp., "backward") sites, i.e., one of the two sites which *are not* on the edge of the cell where the link is missing (resp.,

one of the two sites which *are* on the edge of the cell where the link is missing). We also define $\overline{U}^{(i)}$ as the partition function of the branch restricted to the configurations in which the cell is occupied by a particle in one of the two forward sites, with its "left" (or, equivalently, "right") neighbor cell constrained to be not occupied in one of the two backward sites. Finally, we need to introduce $Z_0^{(i)}$, defined as the partition function of the branch restricted to configurations in which the cell is empty, and $\overline{Z_0}^{(i)}$, corresponding to the partition function of the branch restricted to configurations in which the cell is empty with its "left" (or, equivalently, "right") neighbor cell constrained to be not occupied in one of the two backward sites. Introducing four local cavity fields, defined as $\beta u_i = \ln(U^{(i)}/Z_0^{(i)})$, $\beta d_i = \ln(D^{(i)}/Z_0^{(i)})$, $\beta v_i = \ln(\overline{U}^{(i)}/Z_0^{(i)})$, and $\beta p_i = \ln(\overline{Z_0}^{(i)}/Z_0^{(i)})$, within the RS homogeneous ansatz for the supercooled liquid, the following algebraic recursion relations are derived:

$$
\begin{aligned}
e^{\beta u} &= e^{\beta\mu}T^2 W Z^{-1}, \qquad e^{\beta v} = e^{\beta\mu}T^2 Y Z^{-1} \\
e^{\beta d} &= e^{\beta\mu}T\left(e^{\beta d} + W\right)Y Z^{-1} \qquad (10) \\
e^{\beta p} &= \left[e^{\beta d}\left(W e^{\beta d} + Y\cdot F\right) + Y\left(e^{\beta d} + F\right)W\right]Z^{-1},
\end{aligned}
$$

where $T = e^{\beta p} + e^{\beta v}$, $Y = 1 + 2e^{\beta u}$, $W = 1 + e^{\beta d} + 2e^{\beta u}$, $F = W + e^{\beta d}$, and $Z = \left[e^{\beta d}\left(W e^{\beta d} + Y\cdot F\right) + W^2\left(e^{\beta d} + F\right)\right]$. In terms of the local cavity fields, the contribution to the free energy from the addition of a link between two cells, ΔF_l, and from the addition of a cell, ΔF_s, can be computed:

$$
\begin{aligned}
e^{-\beta\Delta F_l} &= Y^2 + 4e^{\beta d}\left(e^{\beta v} + e^{\beta p}\right) \qquad (11) \\
e^{-\beta\Delta F_s} &= Y\left[4e^{\beta\mu}T^2\left(W + e^{\beta d}\right) + Z\right] + 2e^{\beta(d+p)},
\end{aligned}
$$

from which one can derive the free energy per site $F = (\Delta F_s - 2\Delta F_l)/4$, the density of particles $\rho = \langle n_i \rangle = -(\partial F/\partial\mu)/4$, and the entropy per site $S = -\beta F - \beta\mu\rho$.

The recursion relations for the case $L = 3$ can be determined using a similar procedure. In Fig. 5, the entropy, S, is plotted as a function of the density, ρ, for $L = 1$, $L = 2$ and $L = 3$, in the homogeneous solution for the supercooled liquid. The figure shows that the expansion around the mean-field limit systematically modifies the results. In particular, we note that the density at which the entropy of the supercooled liquid vanishes, $\rho_{S=0}(\sim \rho_K)$, moves toward higher densities when L is increased. As a consequence, the instability of the supercooled liquid (and, therefore, the transition to the glassy phase) is displaced toward the maximum density when bigger two dimensional cells are considered. In fact, we find that $\rho_{S=0}$ approaches very nicely $\rho_{max} = 0.2$ as a power law: $\rho_{S=0}(L) \simeq 0.2 - 0.024\,L^{-0.44}$.

Further insights can be gained by studying the value of the entropy of the supercooled liquid in the zero temperature limit, defined as $S_\infty = \lim_{\mu\to\infty} S$. S_∞ is negative in the mean-field approximation $[S_\infty(L=1) \simeq -0.291]$ and increases systematically as L is increased. We find that
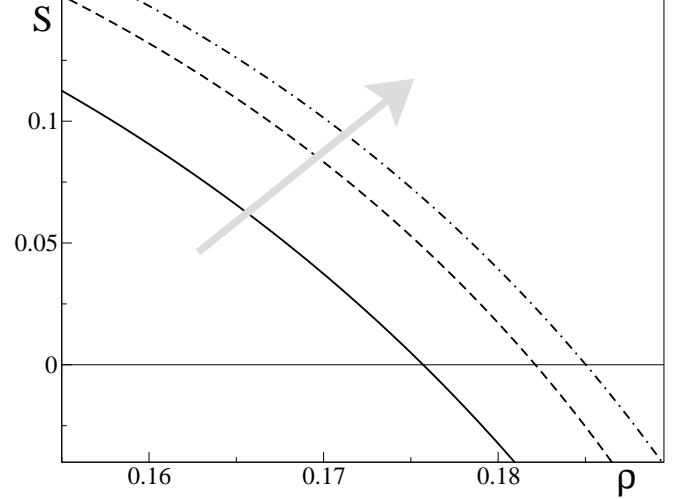

FIG. 5: Entropy per site, S, as a function of the density, ρ. L increases along the direction of the arrow: $L = 1$ (continuous curve), $L = 2$ (dashed curve) and $L = 3$ (dotted-dashed curve). The density at which the entropy of the supercooled liquid vanishes, $\rho_{S=0}$, increases as L is increased.

S_∞ nicely approaches zero as a power law as a function of L: $S_\infty \simeq -0.291\,L^{-0.36}$.

These results clearly hints that the instability of the supercooled liquid and the thermodynamic transition to the glassy phase is smeared out in two dimensions, as one includes corrections to the mean-field theory: the entropy of the supercooled liquid seems to vanish only at the maximum density of the crystalline state. This is in agreement with the recent findings of Refs. [5, 6]. Our results are also in agreement with those of Ref. [7], where, by employing a suitable Monte Carlo algorithm, the authors show that there is no evidence for a thermodynamic phase transition up to very high densities in two dimensional (polidisperse) hard disks; the glass is thus indistinguishable from the liquid on purely thermodynamic grounds. Note, however, that in Ref. [16] the authors state that numerical claims in favour of and/or against a thermodynamic glass transition must be considered carefully, due to the difficulties to probe the system close enough to ρ_K.

If the liquid has to be a good solution in the $L \to \infty$ limit up to ρ_{max}, its pressure must diverge at this point. In fact, we find that for every value of L, the pressure of the supercooled liquid diverges for $\mu \to \infty$, i.e., the entropy of the liquid approaches S_∞ at ρ_{max} with a vertical slope. Since, as discussed above, S_∞ is extrapolated to zero and $\rho_{S=0}$ is extrapolated to ρ_{max} as L is increased, it seems reasonable to expect that in the large L limit the entropy of the liquid vanishes at ρ_{max} and that, consistently, the pressure diverges at this point.

However, it is important to highlight that this is not a *proof* but just a *hint* of the absence of the glass transition in hard disks: as a matter of fact, $\rho_{S=0}$ is only an upper

bound to ρ_K. Thus it might be possible that, in the limit of large L, $\rho_K < \rho_{max}$ even if $\rho_{S=0} \to \rho_{max}$. In principle, one should compute ρ_K for different values of L, by solving the 1RSB equations, which is, unfortunately, a hard numerical task. Nevertheless, given the closeness of ρ_K to $\rho_{S=0}$ for $L = 1$, and the consistency of the liquid solution when extrapolated for large L up to ρ_{max}, one might guess that the possibility described above is unlikely and that $\rho_{S=0}$ provides a good estimation for ρ_K also for bigger L.

In conclusion, we have presented an analytical study of a system of identical hard spheres, focusing on the case of hard disks on a square lattice. The mean-field version on the model exhibits an ideal glass transition of the same kind of that found in mean-field discontinuous spin glasses [8]. Nevertheless, by considering a systematic expansion around the mean-field solution able to take into account short range correlations in an exact fashion, we have shown that such glass transition seems to be smeared out in two dimensions, confirming the results of Refs. [5, 6, 7]. Note that the results presented here are also in agreement with the recently discovered mapping of glass forming system to Ising spin glasses in an external magnetic field [17], according to which there should not be a thermodynamic glass transition in dimensions less than six. Since there cannot be a dynamical glass transition without a thermodynamical one (provided that the dynamics satisfies the detailed balance), we finally argue that there is no structural arrest in two dimensional hard disks at a density smaller than the one of the crystalline packing. This analysis could be generalized to the three dimensional case (which is the most relevant for supercooled liquids) and to higher spatial dimensions, providing a direct way to investigate the lower critical dimensionality of the mean-field ideal glass scenario. This study could prune down the number of candidate theories for the glass transition.

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